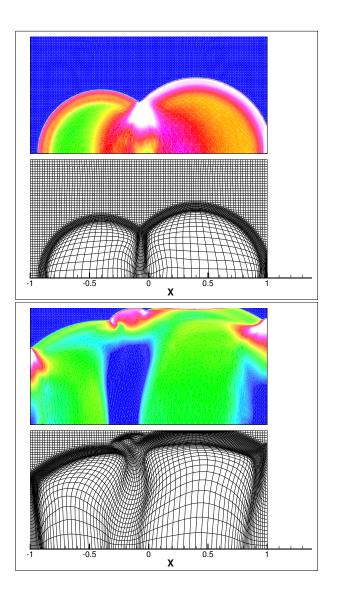
Mathematical Modeling and Analysis



The Repair Paradigm: New Algorithms and Applications to Compressible Flow

Raphaël Loubère loubere@lanl.gov Martin Staley mstaley@lanl.gov Burton Wendroff bbw@lanl.gov

A critical part of Lagrangian-based methods for Computational Fluid Dynamics (CFD) is the ability to remap or interpolate data from one computational mesh to another. This is the case for the popular ALE schemes that perform Lagrangian steps followed by remaps to fixed grids. Remapping is also essential for pure Lagrangian methods, since they can lead to tangled grids that must then be untangled with a concomitant remap step. Even if the basic scheme produces only physically meaningful quantities, a remapping method can create out-of-bounds quantities such as negative densities or pressures. In some CFD codes, the offending values are simply set to a small positive number when this occurs, at which point mass or total energy is no longer conserved. Although in most instances the error thereby created is negligible, we have shown that in at least one example the error is significant. It is possible, by taking great care with the remapping in the CFD context, to maintain positive mass density. This is done by first extending the given mean densities in each original cell to the whole domain so that the new distribution is everywhere positive, and then computing new mean values by exact integration over the cells of the new grid. Total energy can be remapped in this way, but then there is no guarantee that internal energy will be positive. Furthermore, in more than one dimension, exact integration is computationally intensive. Another context in which non-physical data can occur is in divergence-free advection of a concentration that must retain values between zero and one. High quality advection schemes,



Interaction of two blastwaves in a box — Initially two half disks centered at $X = (\pm 0, 5, 0)$ have a high energy compared to the interior of the box — Left picture: t = 0.3, right picture: t = 0.8.

some of which are based on remapping ideas [1], [2], unavoidably have this fault [3]. The goal in this work is to improve upon and apply the repair idea introduced in [4], [5]. A repair method can be viewed as a way to correct values on a discrete mesh by redistributing the conserved quantity so that conservation and a maximum princi-

The Repair Paradigm: New Algorithms and Applications to Compressible Flow

ple are preserved. The maximum principle is that new values should obey certain upper and lower bounds obtained from old values. In this way not only are non-physical quantities eliminated, but oscillations are reduced (albeit not necessarily eliminated). We therefore seek repair algorithms that can be applied to CFD problems, advection problems, or other situations where values of a discrete variable must be placed in bounds without violating a conservation law and without introducing significant errors in the dynamics.

Repair methods can be used for many kinds of variables, including density, velocity, energy, pressure, and concentration. If we denote old cells by c and new cells by \tilde{c} , then the quantity to be conserved is for example the total mass $m = \sum_c m(c) = \sum_c \rho(c) V(c)$, where m(c), $\rho(c)$, and V(c) denote the mass, density, and volume, respectively, of cell c.

Consider an old mesh \mathcal{M} with cell-averaged densities, and a new mesh $\widetilde{\mathcal{M}}$ with remapped cell-averaged densities. The connectivity is the same for the old and new grids, and typically the new mesh is a small perturbation of the old grid. If we define the *bound* neighborhood N(c) of a cell c as a patch of surrounding cells, we can define maximum and minimum density bounds as $\rho_+(c) = \max_{s \in N(c)} \rho(s)$ and $\rho_-(c) = \min_{s \in N(c)} \rho(s)$. (There are other reasonable ways to define density bounds.) No matter how the bounds are defined, there is a feasibility condition for repair to work at all.

The total mass m must not exceed (resp. be below) the total upper bound mass (resp. the total lower bound mass), that is, the total mass if each new cell were at its upper (resp. lower) bound.

If a remapping process produces negative densities, or more generally produces out-of-bounds densities, then a repair step must be done to make these densities obey their bounds. The properties to be fulfilled by a repair method are:

Conservation:

$$\sum_{c} m(c) = \sum_{c} \rho(c) V(c) = \sum_{\tilde{c}} \rho(\tilde{c}) V(\tilde{c}) = \sum_{\tilde{c}} m(\tilde{c})$$

Maximum principle:

$$\forall c, \quad \rho_{-}(c) \leq \rho(\tilde{c}) \leq \rho_{+}(c).$$

In this work we first reviewed a local repair method [5] which repairs out-of-bounds values and distributes the mass discrepancies locally. This method can produce different results depending on the order in which cells are visited, and it is therefore called order-dependent. Next we reviewed a simple global repair process ([4]) which repairs out-of-bounds values and distributes the resulting mass discrepancy across the entire grid. Then we introduced two orderindependent local methods but only one is well suited for parallelization treatment. The idea of this method is to repair as many cell as possible with a local treatment: first the upper bounds (then the lower) with an iterative process (the neighborhood being fixed). Then if some cells are still out-of-bounds a global treatment is provided to fix these cells.

Numerical tests are performed to show the effects of such methods on advection and hydrodynamics problems like the double non-symmetric blastwave solved with an ALE code where the repair method is necessary for the code to produce a physically meaningfull solution (see the figure).

Acknowledgements

Funded by the Department of Energy under contract W-7405-ENG-36 Los Alamos Report LA-UR-04-0795.

References

- P.Colella. Multidimensional upwind methods for hyperbolic conservation laws. *J. Comp. Phys*, 87:171–200, 1990.
- [2] J.K.Dukowicz and J.R.Baumgardner. Incremental remapping as a transport/advection algorithm. *J.Comp.Phys*, 160:318–335, 2000.
- [3] A.Oliveira and A.B.Fortunato. Toward an oscillation-free, mass conservative, eulerian-lagrangian transport model. *J. Comp. Phys.*, 183:142–164, 2002.
- [4] M.Shashkov and B.Wendroff. The repair paradigm and application to conservation laws. *J.Comp.Phys*, 198:265–277, 2004.

Mathematical Modeling and Analysis



- [5] M.Kucharich M.Shashkov and B.Wendroff. An efficient linearity-and-bound-preserving remapping method. *J.Comp.Phys*, 188:462–471, 2003.
- [6] R.Loubere M.Staley and B.Wendroff. The Repair Paradigm: New Algorithms and Applications to Compressible Flow. submitted to J.Comp.Phys, 2004 LAUR-04-XXXX.